

CHAPTER 3

Data Qualifiers

3-1. Introduction.

a. **Data qualification** is an integral component of data review and validation. During PB data review, **data qualifiers** or **flags** are applied to alert the end user to quality problems that may impact the usability of the data (e.g., QC acceptance limits that were not met). However, it is emphasized that data qualification essentially results in a *qualitative* evaluation of the data (e.g., measurement uncertainty is not evaluated in a quantitative manner). This is one of the major reasons why data review or validation is “only a first-step process for the assessment of data usability” (as stated in Chapter 1.2.2).

b. During PB data evaluation, results are either *accepted* or reported with *data qualifiers* or *flags*. Data that meet all QC acceptance limits are *potentially* usable and are *not* qualified. Data that fail one or more QC criteria are qualified as *estimated* (with the *J flag*), *tentatively rejected* (with the *X flag*), or *rejected* (with the *R flag*). The distinction between *estimated*, *tentatively rejected*, and *rejected* data resides in the degree of the QC failure and is *highly dependent upon the reviewer’s understanding of the objectives of the project*.

c. In general, data that are believed to be *completely unusable* with a high degree of confidence (e.g., because of the gross failure of QC criteria) are qualified as *rejected* and would not normally be used to support decisions for an environmental project. Data associated with a *marginal* failure of QC criteria that are believed to be *tentatively usable* or “more usable than not” are qualified as *estimated*. Data that are “mostly unusable” or that fall into the “gray area” between *estimated* and *rejected* are qualified as *tentatively rejected*.

Note: Typically, when data validation is performed, data are primarily qualified as either *estimated* (e.g., with the *J flag*) or *rejected* (e.g., with the *R flag*). However, since data are usually rejected only for the most severe or blatant QC problems, the *R flag* is rarely applied. When QC problems are observed, the data are frequently qualified as *estimated* and are subsequently used to support project decisions. Unfortunately, J-qualified data are often used to support project decisions without evaluating the impact of the QC problems on the usability of the data, resulting in an over estimation of data quality. To minimize the potential indiscriminate use of J-qualified data, an additional data qualifier, the *X flag*, has been defined. During a PB review, depending upon the severity of the QC problem, data are primarily qualified as either “estimated and tentatively accepted” (*J flag*), “estimated and tentatively rejected” (*X flag*) or “rejected” (*R flag*).

d. As stated earlier, full data usability assessment is a more complex and comprehensive activity than data review or validation and is usually performed by the end user (rather than by the data reviewer) because the data user typically possesses a greater understanding of the project’s DQOs (e.g., because of a more extensive knowledge of the project’s history). Therefore, the end user must ultimately determine the acceptability of the data. However, this does not im-

ply that the end user may apply qualified data in an indiscriminate fashion. This is particularly true of data that have been qualified as *tentatively rejected*. *Tentatively rejected data must not be used to support project decisions unless the data user presents (i.e., documents) some technical rationale for doing so.* In other words, *tentatively rejected* data must ultimately be *rejected* (e.g., using the R flag) in the absence of a scientifically defensible rationale to do otherwise. *This requirement should be explicitly specified in the QAPP.* Furthermore, when data qualified as *tentatively rejected* are used to support decisions for a project, the data reviewer should be consulted for a consensus unless it is clear that the reviewer did not possess a complete understanding of the objectives of the investigation (e.g., new DQOs were established after the data review was performed). It should be noted “Chemical Data Quality Assessment Reports” (as defined by EM 200-1-6, 10 October 1997) by USACE project chemists represent one possible mechanism to document a more comprehensive usability evaluation (e.g., X-flagged data may be converted to J-flagged or R-flagged data in Chemical Data Quality Assessment Reports).

e. Ideally, *estimated* (i.e., J-qualified) data, though presumed to be usable by the data reviewer, should be accepted by the end user only after the reasons for the data qualifications and their impact on the achievement of project DQOs have been examined. For example, when the direction of bias and the magnitude of the analytical uncertainty are well defined, a more thorough examination of the data may entail an evaluation similar to that presented in Paragraph 11-6.

3-2. Definitions of Data Qualifiers.

a. All data qualifiers or flags must be clearly defined. Project-specific requirements ultimately determine the types of qualifiers that are required (e.g., the EPA Functional Guidelines for validation require a distinct set of flags). However, in the absence of more appropriate conventions for data qualification, the flags defined below must be used. The definitions of the data qualifiers are summarized in Table 3-1.

(1) *R flag.*

(a) The datum is rejected. The qualifier typically indicates that a datum is completely unusable because it is of unknown quality (e.g., missing QC information) or because of gross QC deficiencies (e.g., extremely poor recoveries for the LCS).

(b) NFor gas chromatography/mass spectrometry (GC/MS) analyses, the R flag must be used to reject TIC tentatively identified compound results that are believed to be laboratory artifacts (i.e., common laboratory contaminants). Examples include reagent contaminants, solvent preservatives, siloxanes, and aldol condensation reaction products of acetone (e.g., 4-hydroxy-4-methyl-2-pentanone, 4-methyl-2-penten-2-one, and 5,5-dimethyl-2(5H)-furanone).

(2) *J flag.* The target analyte is *positively identified*, but the reported numerical result (e.g., analyte concentration) is an *estimated* value and the direction of bias is unknown. The flag indicates that a significant *quantitative* (as opposed to a qualitative) uncertainty exists. The J flag must *always* be used to report the following.

(a) Detections below the **method quantitation limit (MQL)**.

(b) Tentatively Identified Compounds (TICs).¹

(3) *J-Flag*. The target analyte is present but the reported numerical result is an estimate that is believed to be *biased low* (e.g., the actual concentration in the environmental sample is believed to be *greater* than the reported concentration).

(4) *J+ Flag*. The analyte is present but the reported numerical result is an estimate that is believed to be *biased high* (e.g., the actual concentration in the environmental sample is believed to be *less* than the reported concentration).

(5) *N Flag*. The target analyte is reported as a *tentative detection* (e.g., because the identity of the analyte is in doubt). The N flag indicates a significant *qualitative* rather than quantitative uncertainty exists (i.e., the reported detection of the analyte may be a “false positive”). When used in combination with the U flag (i.e., the UN flag), the qualifier indicates that the absence of a target analyte at some stated reporting limit is in doubt (i.e., a false negative is possible at the stated reporting limit). Applications of the N flag include the following:

(a) Uncertain Aroclor identifications (e.g., weathered PCBs).

(b) Tentatively Identified Compounds.

(6) *U Flag*. The analyte was not detected relative to the **method reporting limit (MRL)**; that is, the result is less than the method reporting limit (MRL).

(7) *NJ Flag*. The presence or identity of the analyte is in doubt and the reported concentration is estimated. The estimation is both *qualitative and quantitative* in nature.

(8) *UN Flag*. The result is reported as a *tentative nondetection* (as opposed to tentative detection); there is uncertainty with whether or not the nondetection is valid at the stated method reporting limit (e.g., because of QC problems).

Note: The UN flag is similar (but not identical) to the CLP “UJ flag,” which is defined as follows: “The analyte was not detected above the reported sample quantitation limit. However, the reported quantitation limit is approximate and may or may not represent the actual limit of quantitation necessary to accurately and precisely measure the analyte in the sample.” Both flags indicate that an uncertainty is associated with a nondetection. However, the UJ and UN flags differ in that the former is defined in terms of the CLP CRQLs, while the latter is defined in terms of *project-specific reporting limits*. The UN and UJ qualifiers are essentially equivalent when the reporting limits equal the CRQLs. However, in general, setting the reporting limits equal to the quantitation limits is not recommended (e.g., unless the action levels for the project are high).

¹ TICs are typically qualified by the laboratory.

(9) *X Flag*. The datum is *tentatively rejected* because project-specific data quality objectives (e.g., for sensitivity, accuracy, or precision) were not met or were not demonstrated. When objectives for sensitivity are not met, the X flag typically indicates that a result (a detection or nondetection) is potentially unusable with respect to an action level (e.g., the result does not demonstrate that a target analyte is actually present in an environmental sample at a concentration above or below a risk-based decision limit).

Note: When evaluating objectives for sensitivity, the R flag may be more appropriate than the X flag when action levels are fixed and statistical analyses are not being performed. The X flag may be appropriate when action levels are subject to change, a set of data is being evaluated with respect to different action levels, or when statistical analyses are being performed.

b. It may be desirable to use the X flag in combination with other flags as illustrated below:

(1) *X- Flag*. The detection is (quantitatively) grossly estimated with low bias and is tentatively rejected.

(2) *X+ Flag*. The detection is (quantitatively) grossly estimated with high bias and tentatively rejected.

(3) *XN Flag*. The detection is quantitatively and qualitatively highly estimated and is tentatively rejected.

(4) *XU Flag*. The nondetection is tentatively rejected.

c. When a datum is qualified, the reviewer must explain *why* the particular qualifier was applied. It is recommended that numerical subscripts be placed on flags to indicate why the flag was used (e.g., the flags J₁ and J₂ may indicate that a result is estimated because of poor target analyte **recovery** for the associated laboratory control sample and matrix spike, respectively). However, the use of subscripts may not be practical for projects that involve a large number of samples when the samples possess multiple QC problems. Similarly, it may be desirable to suppress the numerical subscripts when the reasons why the flags were applied are not important to a particular data user. However, the rationale for each qualification must be explained in the data review report.

d. When possible, the J flag must identify any suspected bias (high or low) in the data. If bias is known for an estimated result, use either the J- or J+ flag to qualify a result. However, if a datum is estimated because of multiple QC problems and the direction of bias is not well defined, it may be appropriate to qualify the datum as *tentatively rejected* rather than as *estimated*.

Table 3-1
Summary of Major Data Qualifiers

Qualifier	Definition
J	Estimated (quantitatively) and tentatively usable
J-	Estimated (quantitatively) with low bias
J+	Estimated (quantitatively) with high bias
U	Below reporting limit
N	Qualitatively estimated (tentative detection)
X	Tentatively rejected
R	Rejected
UN	Tentative nondetection
NJ	Quantitatively and qualitatively estimated